

Isobutyl nitrite
542-56-3 | DTXSID3020750

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 21.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.83e-01

Confidence level: 6.21e-01

Nearest Neighbors from the Training Set

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1-Pentanol

Measured: 5.01

Predicted: 7.31

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Toluene

Measured: 117

Predicted: 87.4

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Phenol

Measured: 26.9

Predicted: 57.3

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Resorcinol

Measured: 9.55

Predicted: 28.3

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Anisole

Measured: 34.7

Predicted: 69.5